CS 357: Numerical Methods

Singular Value Decomposition
Rank-K Approximations
Total Least Squares

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Computing the SVD

$A = U \Sigma V^T$ $\qquad$ A $m \times n$

① Find V $\qquad$ $A^T A v_i = \lambda_i v_i$ $\qquad$ V $n \times n$

$$V = \begin{bmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{bmatrix}$$

② Form Σ $\qquad$ Σ $m \times n$

$$\begin{bmatrix} \sqrt{\lambda_1} & & 0 \\ & \ddots & \\ 0 & & \sqrt{\lambda_n} \end{bmatrix}$$

Computing the SVD

$A = U \Sigma V^T$

$AV = U \Sigma$

if A $n \times n$

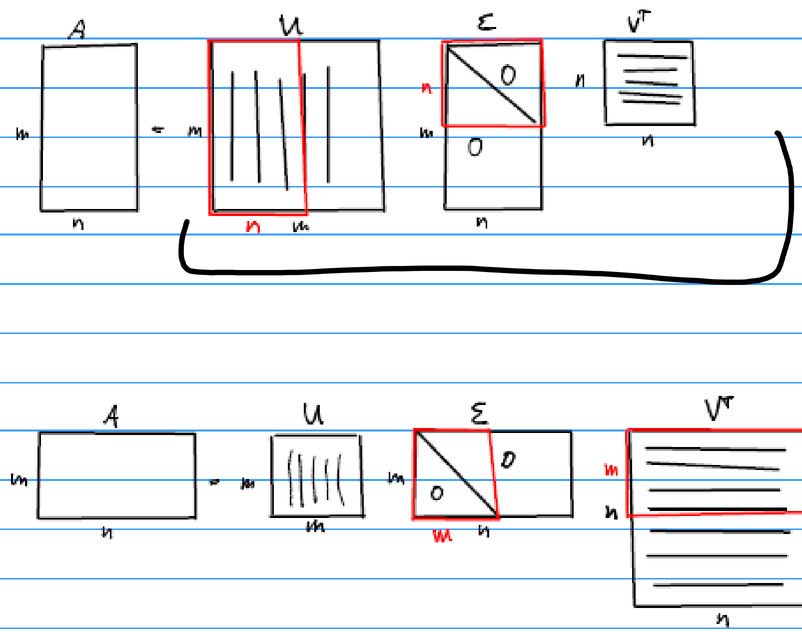
$$AV\Sigma^{+} = U \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix}$$

Pseudoinverse of Σ

$$\Sigma = \begin{array}{cc} & n \\ m & \begin{bmatrix} \ddots & \\ & \\ & \end{bmatrix} \end{array} \qquad \Sigma^{+} = \begin{bmatrix} \ddots & & \end{bmatrix}$$

$$\Sigma^{+} = \begin{bmatrix} 1/\sqrt{\lambda_1} & & \\ & \ddots & \\ & & 1/\sqrt{\lambda_n} \end{bmatrix}$$

Reduced Form of the SVD



"Full" version shown in black

"Reduced" version shown in red

Rewriting the SVD

$$A = U \Sigma V^T = \begin{pmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} - & v_1 & - \\ & \vdots & \\ - & v_n & - \end{pmatrix}$$

$$A = \Sigma \, \sigma_i \underbrace{u_i v_i^T}_{\text{outer product}}$$

$$\underset{2\times 1}{\begin{pmatrix} 2 \\ 4 \end{pmatrix}} \underset{1\times 2}{\begin{pmatrix} 1 & 3 \end{pmatrix}} = \begin{pmatrix} 2 & 6 \\ 4 & 12 \end{pmatrix}$$

Rank-K Approximations

X is a set of 2D points

$X = \begin{pmatrix} | & & & | \\ x_1 & \cdot & \cdots & x_n \\ | & & & | \end{pmatrix}$ n points

x_i is the ith point

$\underbrace{X}_{2\times n} = \underbrace{U}_{2\times 2}\ \underbrace{\Sigma}_{2\times 2}\ \underbrace{V^T}_{2\times n}$

u_1 first col of u

σ_1 top σ in Σ

v_1^T first row v^T

For Rank-1 approx

$$\boxed{X \approx u_1 \sigma_1 v_1^T = X_1}$$

Rank-K Approximations

Frobenius Norm

$$\|X\|_F = \sqrt{x_{11}^2 + x_{12}^2 + \cdots + x_{mn}^2}$$

$\|X - B\|_F^2$ is minimized by $B = X_1$ where B is rank 1 matrix

$$\|X - X_1\|_F^2 = \sum \| x_j - \underbrace{u_1 \sigma_1 v_j}_{\text{scalar multiple of vector } u_1} \|_2^2$$

Rank-K Approximations

v_1 from V is eigenvector of A^TA
u_1 from U is principal e.vec of AA^T

Rank-2 approximation finds
2 vectors spanning a plane
having minimal distance to
datapoints

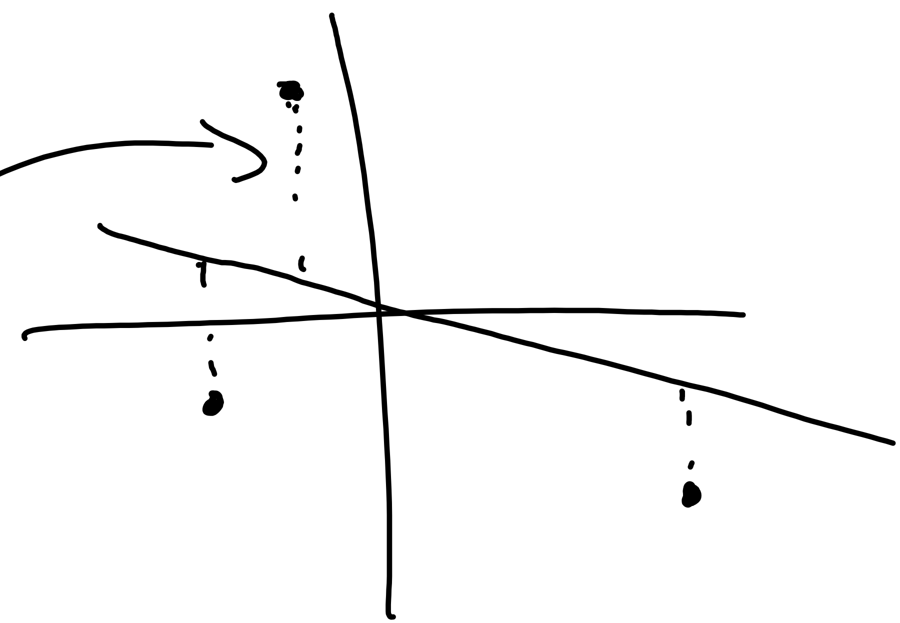
Total Least Sqaures

$(t_i, y_i) = (-2, -1)$

$(-1, 3)$

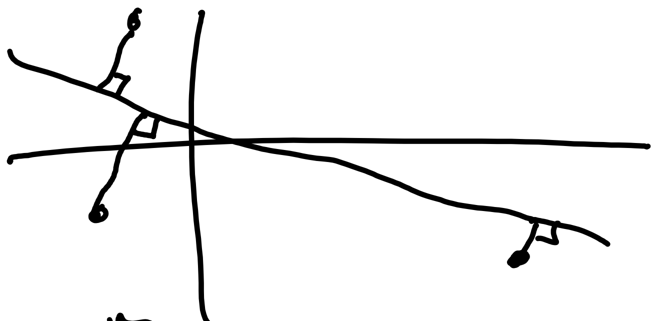
$(3, -2)$

Linear
Least
Squares
minizes
vertical
distances



Total Least Sqaures

Imagine points (t_i, y_i) have error in both t_i and y_i



minimize dist perp. to line

"ordinary least squares" $Ax \cong b$

we want to find $\tilde{x}$

$\underbrace{A\tilde{x} = y}$ and

$\|b - y\|_2$ is minimal

and $y \in \text{span}(A)$

Total Least Sqaures

Ordinary least squares $b \approx y$ $\quad Ax \approx b$

$\longrightarrow$ RHS varies $\quad \hat{A}x = y$

For total least squares

A varies as well

$[Ab] = U\Sigma V^T \longrightarrow m \times (n+1)$

find $[\hat{A}y]$ approximates $[Ab]$

$\hookrightarrow y \in \operatorname{span} \hat{A}$

Total Least Sqaures

Use rank n approx. of $\underset{\sim}{[}Ab]$

$$\boxed{\hat{A}x = y}$$

$$[\hat{A}\; y] \begin{bmatrix} x \\ -1 \end{bmatrix} = 0$$

$\rightarrow [x^T \; -1]^T$ is in nullspace $[\hat{A}\; y]$

$\rightarrow [x^T - 1]$ proportional to v_{n+1}

$=$

$$\boxed{x = -\frac{1}{v_{n+1,n+1}} \begin{bmatrix} v_{1,n+1} \\ \vdots \\ \vdots \\ v_{n+1,n+1} \end{bmatrix}}$$

$$[A\ b] = U \Sigma V^T$$

$v_{n+1} \Rightarrow$ last col V